

# THE MERCK INDEX

THIRTEENTH EDITION

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AN ENCYCLOPEDIA OF  
CHEMICALS, DRUGS, AND BIOLOGICALS

THIRTEENTH EDITION

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**4911. Idarubicin.** [58957-92-9] (7S,9S)-9- $\beta$ -D-amino-2,3,6-trideoxy- $\alpha$ -L-( $\gamma$ -xohexopyranosyl)oxy-10-tetrahydro-6,9,11-trihydroxy-5,12-naphthacenedione-3-acetyl-1,2,3,4,6,11-hexahydro-3,5,12-trihydroxy-1-naphthacenyl-3-amino-2,3,6-trideoxy- $\alpha$ -L-xylopyranoside; 4-demethoxydaunomycin; 4-demethoxydaunorubicin; DMDR; IMI-30; NSC-256439.  $C_{26}H_{27}NO_{10}$ . 497.49. C 62.77%, H 5.47%, N 2.82%. O 28.94%. Optical activity:  $[\alpha]_D^{25} +10.5$  (c 0.5, CHCl<sub>3</sub>). Infrared (KBr): 3400 (broad), 1650, 1550, 1500, 1450, 1380, 1350, 1280, 1250, 1180, 1150, 1100, 1050, 1020, 1000, 950, 900, 850, 820, 800, 750, 720, 700, 650, 620, 600, 550, 520, 500, 450, 420, 400, 350, 320, 300, 250, 220, 200, 180, 150, 120, 100, 80, 60, 40, 20, 10, 0. Proton magnetic resonance (CDCl<sub>3</sub>):  $\delta$  7.2-7.8 (m, 8H, aromatic), 6.2-6.8 (m, 4H, aromatic), 5.2-5.8 (m, 4H, sugar), 4.2-4.8 (m, 4H, sugar), 3.2-3.8 (m, 4H, sugar), 2.2-2.8 (m, 4H, sugar), 1.2-1.8 (m, 4H, sugar), 0.2-0.8 (m, 4H, sugar). Mass spectrometry (EI):  $m/z$  497.49 (M<sup>+</sup>), 479.49 (M<sup>+</sup>-18), 461.49 (M<sup>+</sup>-36), 443.49 (M<sup>+</sup>-54), 425.49 (M<sup>+</sup>-72), 407.49 (M<sup>+</sup>-90), 389.49 (M<sup>+</sup>-108), 371.49 (M<sup>+</sup>-126), 353.49 (M<sup>+</sup>-144), 335.49 (M<sup>+</sup>-162), 317.49 (M<sup>+</sup>-180), 299.49 (M<sup>+</sup>-198), 281.49 (M<sup>+</sup>-216), 263.49 (M<sup>+</sup>-234), 245.49 (M<sup>+</sup>-252), 227.49 (M<sup>+</sup>-270), 209.49 (M<sup>+</sup>-288), 191.49 (M<sup>+</sup>-306), 173.49 (M<sup>+</sup>-324), 155.49 (M<sup>+</sup>-342), 137.49 (M<sup>+</sup>-360), 119.49 (M<sup>+</sup>-378), 101.49 (M<sup>+</sup>-396), 83.49 (M<sup>+</sup>-414), 65.49 (M<sup>+</sup>-432), 47.49 (M<sup>+</sup>-450), 29.49 (M<sup>+</sup>-468), 11.49 (M<sup>+</sup>-486). UV spectrum (CHCl<sub>3</sub>):  $\lambda_{max}$  260 nm ( $\epsilon$  10,000),  $\lambda_{min}$  280 nm ( $\epsilon$  1,000). Biological activity: Antitumor activity: *in vivo* (mouse, L1210 leukemia): ID<sub>50</sub> 0.05 mg/kg (i.p.). *in vitro* (human, L1210 leukemia): IC<sub>50</sub> 0.05  $\mu$ M (i.p.). Toxicity: LD<sub>50</sub> 0.05 mg/kg (i.p.). Synthesis: M. J. Broadhurst *et al.*, *J. Chem. Soc. Chem. Commun.* **1982**, 158. Synthesis of optically pure isomer: M. J. Broadhurst *et al.*, *Bull. Chem. Soc. Japan*, **59**, 423 (1986).